

APPENDIX D

ADVANCED MODELING APPROACHES FOR CHARACTERIZING VARIABILITY AND UNCERTAINTY

D.0 INTRODUCTION

This appendix briefly describes the following advanced modeling approaches that can be used in probabilistic risk assessment (PRA) to characterize variability and uncertainty: two-dimensional MCA (2-D MCA), microexposure event analysis (MEE), geospatial statistics, and Bayesian analysis. Except for 2-D MCA, these approaches can also be applied to point estimate risk assessment. The application of many of these approaches will require access to expertise in specialized areas of statistics and, in some cases, specialized or even custom-designed computer software. The intent here is to introduce some of the basic concepts and terminology, as well as to provide references where the reader can find more exhaustive coverage of these topics.

D.1.0 EXPRESSING VARIABILITY AND UNCERTAINTY SIMULTANEOUSLY

A Monte Carlo analysis that characterizes either uncertainty or variability in each input variable (see Chapter 1) can be described as a one-dimensional Monte Carlo analysis (1-D MCA). A 2-D MCA is a term used to describe a model that simulates both uncertainty and variability in one or more input variables. All probability distributions that are used to describe variability in a PRA model have a certain degree of associated uncertainty. For example, suppose variability in soil concentration (ppm) is estimated using a normal probability density function (PDF) defined by a mean ($\mu_{\text{soil}}=5$) and standard deviation ($\sigma_{\text{soil}}=1$), and subjectively truncated (min, max) at (0, 50). Uncertainty in the parameter estimates can be represented in a PRA model by assuming both parameters are also random variables. To illustrate this concept, assume normal PDFs for *uncertainty* can be specified for both parameters. Uncertainty in the mean is described by the normal PDF with parameters ($\mu_{\text{mean}}=5$, $\sigma_{\text{mean}}=0.5$); similarly, uncertainty in the standard deviation is described by the normal PDF with parameters ($\mu_{\text{SD}}=1$, $\sigma_{\text{SD}}=0.5$). Model variables are represented in this manner when there is a compelling reason to believe that a unique probability distribution does not adequately describe one's knowledge of each variable in the model. A variable described in this way is called a second order random variable. Figure D-1 (Panel A) shows a collection of $n=20$ cumulative probability distributions (CDFs), each curve representing a unique set of (mean, SD) parameter estimates for the normal PDF for variability. Panel B shows the 90% *confidence interval*¹ based on 2,500 simulated CDFs. The 95% lower and upper bounds correspond to the distribution of 5th percentiles and 95th percentiles, respectively (i.e., CDF for 2,500 5th percentiles and CDF for 2,500 95th percentiles). The 90% credible interval (CI) for the 50th percentile is (3.4, 6.7).

¹Note that the term "credible interval" may be more appropriate than "confidence interval" given that the range is based on subjective as well as statistical considerations. Brattin, Barry, and Chiu (1996) provide additional examples of uncertain PDFs that illustrate this concept.

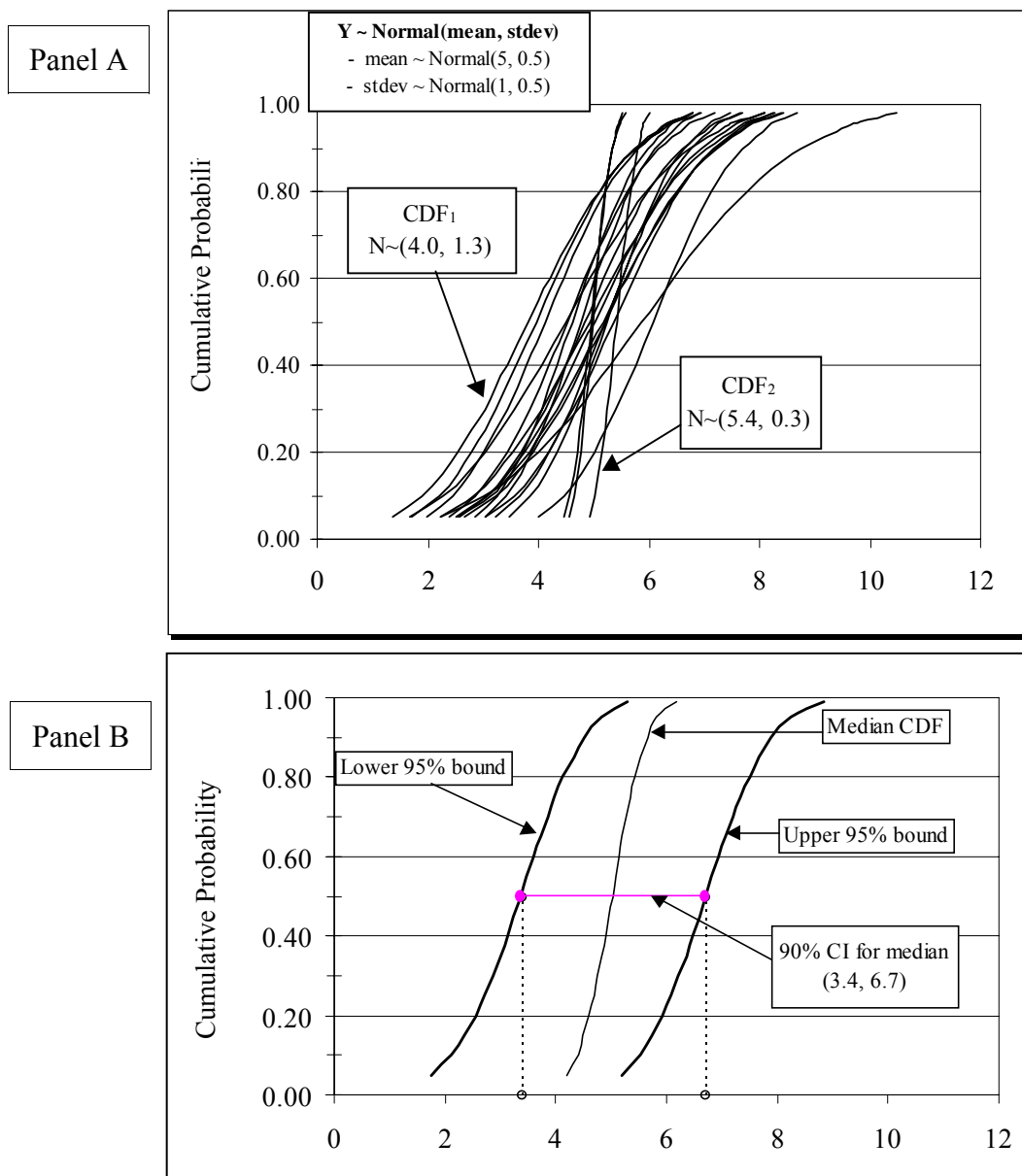


Figure D-1. Panel A shows a family of 20 CDFs for a hypothetical random variable, Y (e.g., concentration in units of ppm), characterized by a normal PDF where both the mean and SD are also random variables representing uncertainty in the parameter estimates: $\text{Mean} \sim \text{Normal}(5, 0.5)$, $\text{SD} \sim \text{Normal}(1, 0.5)$. Each CDF represents a single simulation of $n=2500$ iterations using a unique set of parameters. For example, CDF_1 represents $N \sim (4.0, 1.3)$ while CDF_2 represents $N \sim (5.4, 0.3)$. **Panel B** shows the “90% credible interval” for the CDF based on 2,500 simulations, each simulation using $n = 2500$ iterations (i.e., a 2-D MCA with 2,500 outer loop iterations and 2,500 inner loop iterations). Lower, median, and upper bounds represent the simulated 5th, 50th, and 95th percentiles, respectively. The 90% confidence interval for the estimate of the 50th percentile is: {3.4, 6.7}.

EXHIBIT D-1

DEFINITIONS FOR APPENDIX D

Bayesian Statistics - A specialized branch of statistics that views the probability of an event occurring as the degree of belief or confidence in that occurrence.

Geospatial Statistics - A specialized branch of statistics that explicitly takes into account the georeferenced context of data and the information (i.e., attributes) it contains.

Frequentist - A term referring to classical statistics in which the probability of an event occurring is defined as the frequency of occurrence measured in an observed series of repeated trials.

Image Analysis - A technique in geostatistics used to restore a degraded image or interpret images that have been contaminated by noise or possibly some nonlinear transformation.

Kriging - A geostatistical method of spatial statistics for predicting values at unobserved locations.

Likelihood Function - A Bayesian term referring to a probability distribution expressing the probability of observing a piece of new information given that a particular prior belief is true.

Location Tag - The spatial coordinates of a sampling location (e.g., longitude, latitude).

Microexposure Event Analysis (MEE) - An approach to modeling exposure in which long-term exposure of an individual is simulated as the sum of separate short-term exposure events.

Point Pattern Analysis - A technique in geostatistics of restricting the analysis to location information, ignoring attribute information, addresses two location problems: (1) describing points according to spacing, and (2) describing points according to density.

Posterior Distribution - A Bayesian term referring to a probability distribution that has been updated with new information.

Prior Distribution - A Bayesian term referring to the hypothesized, expected, or calculated probability distribution for an event prior to the collection of new information.

Spatial Autocorrelation - The tendency of data from locations that are relatively close together to be geographically correlated.

Thiessen (Voronoi) Polygon Analysis - A method of spatial statistics in which an area is subdivided into subregions, or polygons, in order to predict values at unobserved locations.

Time Step - A modeling term used to describe the time interval within which variable values do not change.

Two-Dimensional Monte Carlo analysis (2-D MCA) - Separate representation of variability and uncertainty in an MCA, usually accomplished using nested computation loops.

In the example shown in Figure D-1, the mean and standard deviation for soil concentration were allowed to vary independently. Thus, a distribution could be defined by a combination of a low mean and a high standard deviation, high mean and low standard deviation, or any other combination in between. The assumption of independence of variable parameters may not be valid in all cases. It may be unreasonable to assume that a high mean soil concentration would occur with a low standard deviation. An alternative assumption would be that the standard deviation of the mean is a constant proportion of the mean (i.e., a constant coefficient of variation). Correlations between parameters should be considered in the design of the PRA. One approach that is especially useful for characterizing relationships between the slope and intercept of a simple linear regression is to specify the bivariate normal distribution for the parameter estimates.

D.2.0 TWO-DIMENSIONAL MONTE CARLO ANALYSIS (2-D MCA)

Two-dimensional MCA is an approach for computing risk (or hazard) when combining distributions that represent variability and uncertainty. In 2-D MCA, distributions representing variability and uncertainty are sampled using nested computational loops (Figure D-2). The inner loop simulates variability by repeatedly sampling values for each variable from their defined probability distributions. With each circuit of the outer loop, new parameter values for each variable are selected, and the inner loop sampling is repeated. The result is a collection of inner loop simulations, one for each parameter value selected. If the inner loop samples 5,000 times, and the outer loop samples 1,000 times,

then each variable is sampled 5,000,000 times and 1,000 simulated probability distributions of risk are generated from the PRA model. These probability distributions can be analyzed to estimate the distributions for specific risk estimates. For example, confidence limits on the estimate of specific risk percentiles can be simulated using 2-D MCA (Figure D-3).

Simulation Logic for 2-Dimensional MCA

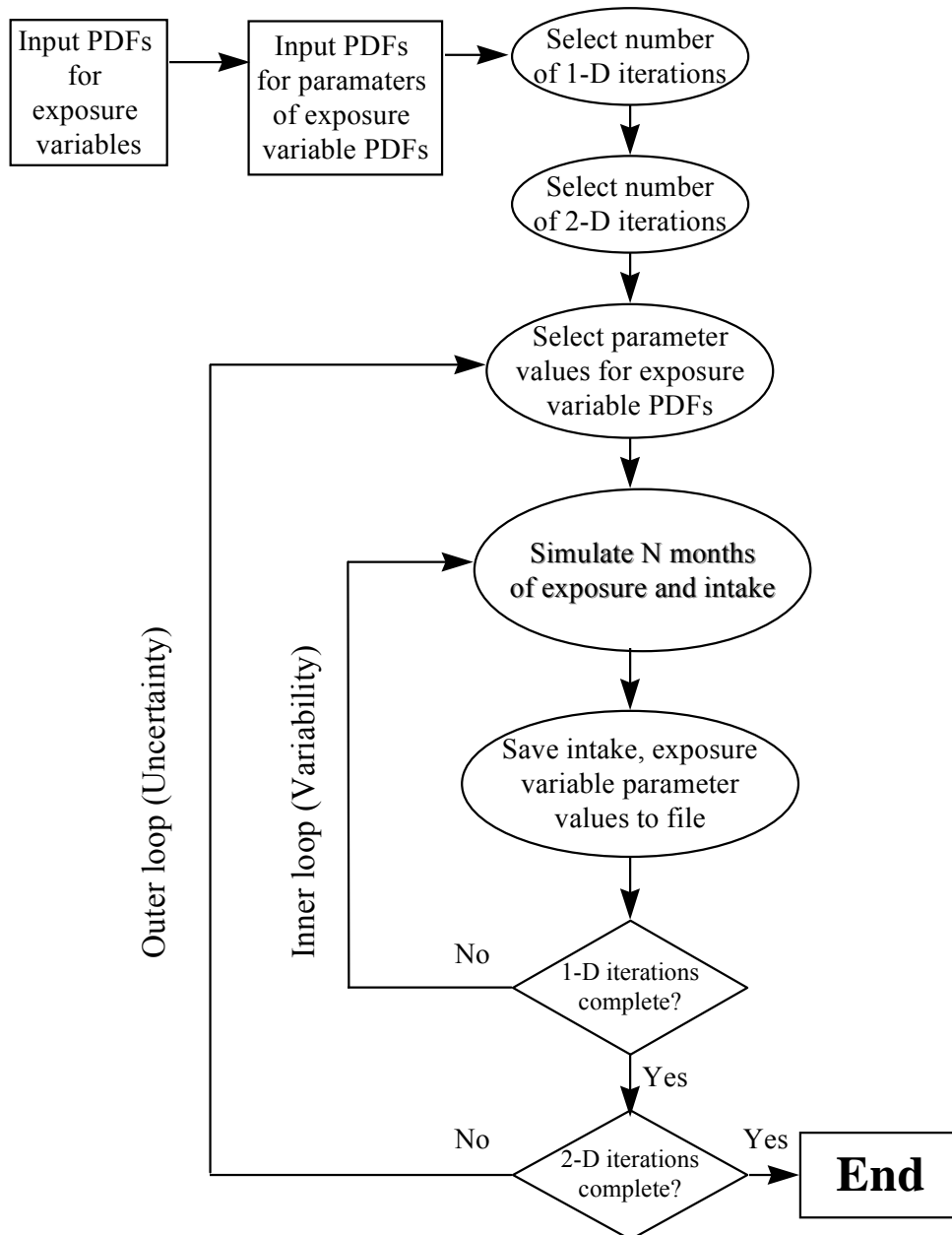


Figure D-2. Diagram showing of a 2-D Monte Carlo model in which the variability and uncertainty dimensions are computed in nested loops. In this example, values for exposure variables in the inner loop represent monthly averages.

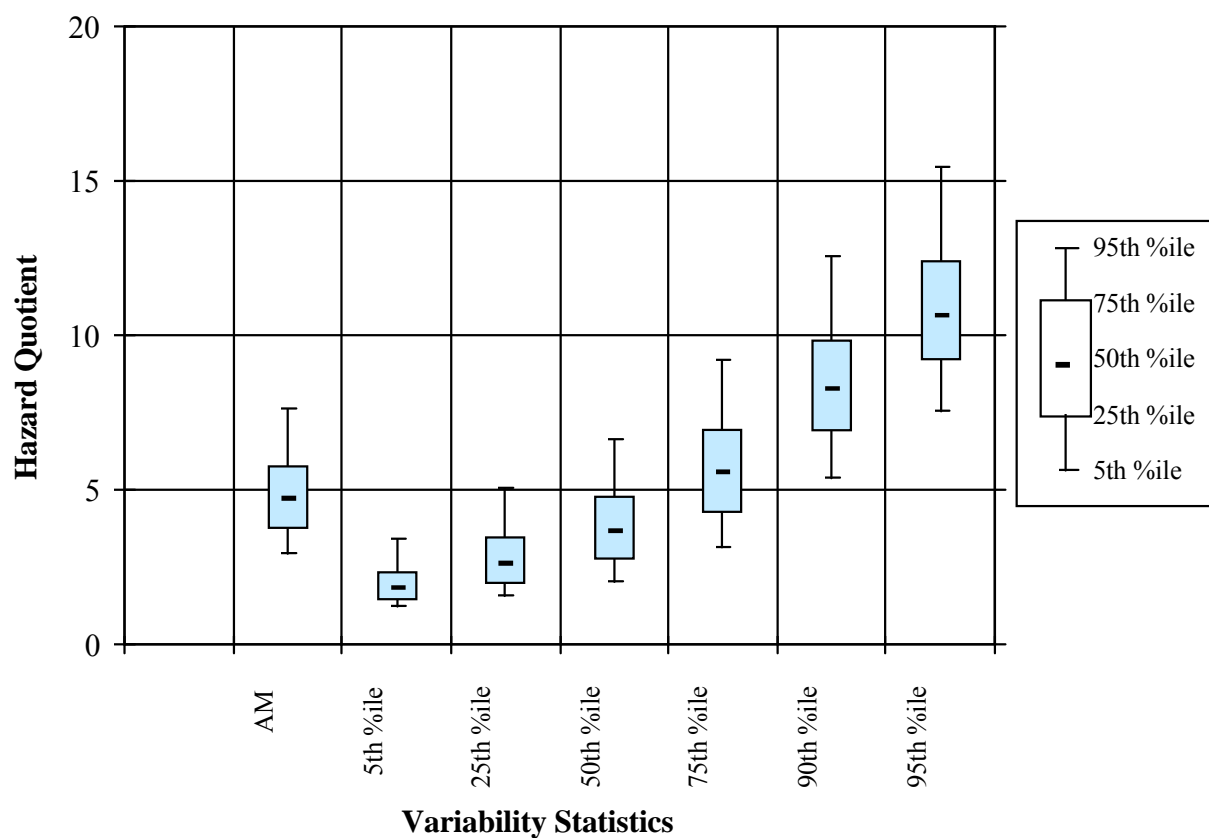


Figure D-3. Output from a 2-D MCA showing the estimated mean Hazard Quotient (HQ) and the 90% confidence interval for the arithmetic mean (AM) and selected percentiles of the HQ distribution. The 95th %ile HQ would be the reasonable maximum exposure (RME) risk estimate. The simulation suggests that there is a 95% probability that the RME HQ (95th percentile) is below 16.

D.3.0 MICROEXPOSURE EVENT ANALYSIS

The standard dose equation generally used in Superfund site risk assessments represents exposures averaged over a specified time period that is relevant to the health endpoint of concern (Equation D-1). If the risk assessment is directed at assessing life-time risk to humans, the averaging time used in Equation D-1 would generally be 70 years (i.e., estimated average human lifetime), and the calculated chemical intake would generally represent the life-time average daily dose (LADD). Where information is available to characterize variability on a smaller time scale than life-time, an alternative expression of dose that accommodates such variability may be desirable.

Concentrations in various environmental media can be expected to vary over time. For example, wind erosion may change chemical concentrations in surface soil. Leaching may change concentrations in both subsurface soil and groundwater. The change in the concentration term is most readily apparent when considering anglers harvesting fish. If an angler consumes a large amount of fish from a single location (e.g., a specific lake, pond, or river), then the average chemical concentration in the fish consumed by that angler can be expected to be similar to the average of the chemical concentration of fish in the population. However, if an angler consumes fish only occasionally, or harvests fish from different locations, there will be considerably more uncertainty in the concentration term. In addition, a harvesting angler may consume varying amounts of fish over the period of the exposure duration due to changing tastes, changes in the fish population size or other factors.

Daily activity patterns, food intake, soil ingestion and other behavioral factors are measured in a time period of less than a year. The extrapolation of these short term results to the chronic exposure situation is a source of uncertainty. Exposure events are real but unknowable, whereas data regarding the nature and magnitude of these events is known but its application to a real world situation is uncertain. Microexposure event analysis (MEE) attempts to explicitly quantify this uncertainty. Figure D-5 presents the general approach for MEE analysis. (Price et al., 1996, 2000). MEE modeling provides an alternative to the standard time-averaging approach represented by Equation D-1. In the MEE approach, long term intake is viewed as the sum of individual exposure events (Equation D-2). Implementing the MEE approach in a PRA requires dividing the exposure duration into short epochs, or time steps, within which the values assigned to exposure variables remain constant, but are allowed to vary from one time step to the next. In a PRA model, exposure variables are adjusted at each time step by selecting values from the probability distributions representing each variable (Figure D-4). Discussion of the

Standard Time-Averaging

$$\text{DOSE} = \frac{C \times \text{IR} \times \text{EF} \times \text{ED}}{\text{BW} \times \text{AT}} \quad \text{Equation D-1}$$

Microexposure Event Modeling

$$\text{DOSE} = \frac{1}{\text{AT}} \sum_{j=1}^{\text{ED}} \frac{1}{\text{BW}_j} \sum_{i=1}^{\text{Events}_j} C_{ij} \cdot \text{IR}_{ij} \quad \text{Equation D-2}$$

C = Concentration; I = exposure event; j = year of life
IR = Intake Rate
EF = Exposure Frequency
ED = Exposure Duration
BW = Body Weight
AT = Averaging Time

implementation of MEE analysis in risk assessment and its merits and limits can be found in Wallace et al. (1994), Price et al. (1996), Slob (1996), and Buck et al. (1997).

In MEE modeling, the time step becomes an important variable, with associated uncertainty. The time step should be selected based on information available to describe how exposures change over time. For example, a model of a moving plume of solvents in groundwater might suggest that chemical concentrations in a given location are dropping by between 16 and 25% quarterly. Several rounds of sampling may support this prediction. This rapid decline in concentrations suggests that an appropriate time step might be one quarter (i.e., three months).

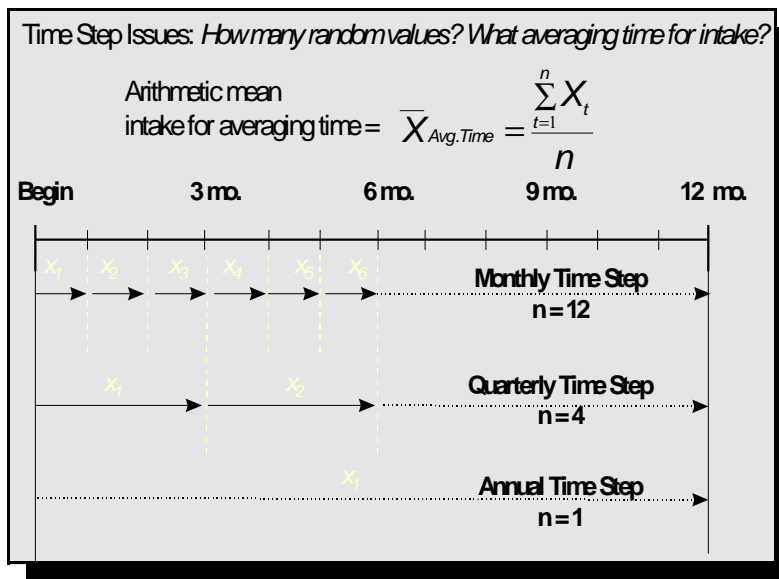


Figure D-4. Time Step for MEE.

On the other hand, where risk is being assessed for metals, dioxin, or PAHs in soil, the concentrations might be expected to change much more slowly, if at all, and the basis of the time step might be the increase in age and corresponding changes in behavior of the receptor. The time step may be global; that is, one time step may apply to all variables in the model. In this case, the same number of random values would be selected for each exposure variable in a Monte Carlo simulation. A more complex model may use different time steps for different variables, requiring some probability distributions to be sampled more often than others. The selection of a value for a time step implies that the value represents the average value for that variable during the time step.

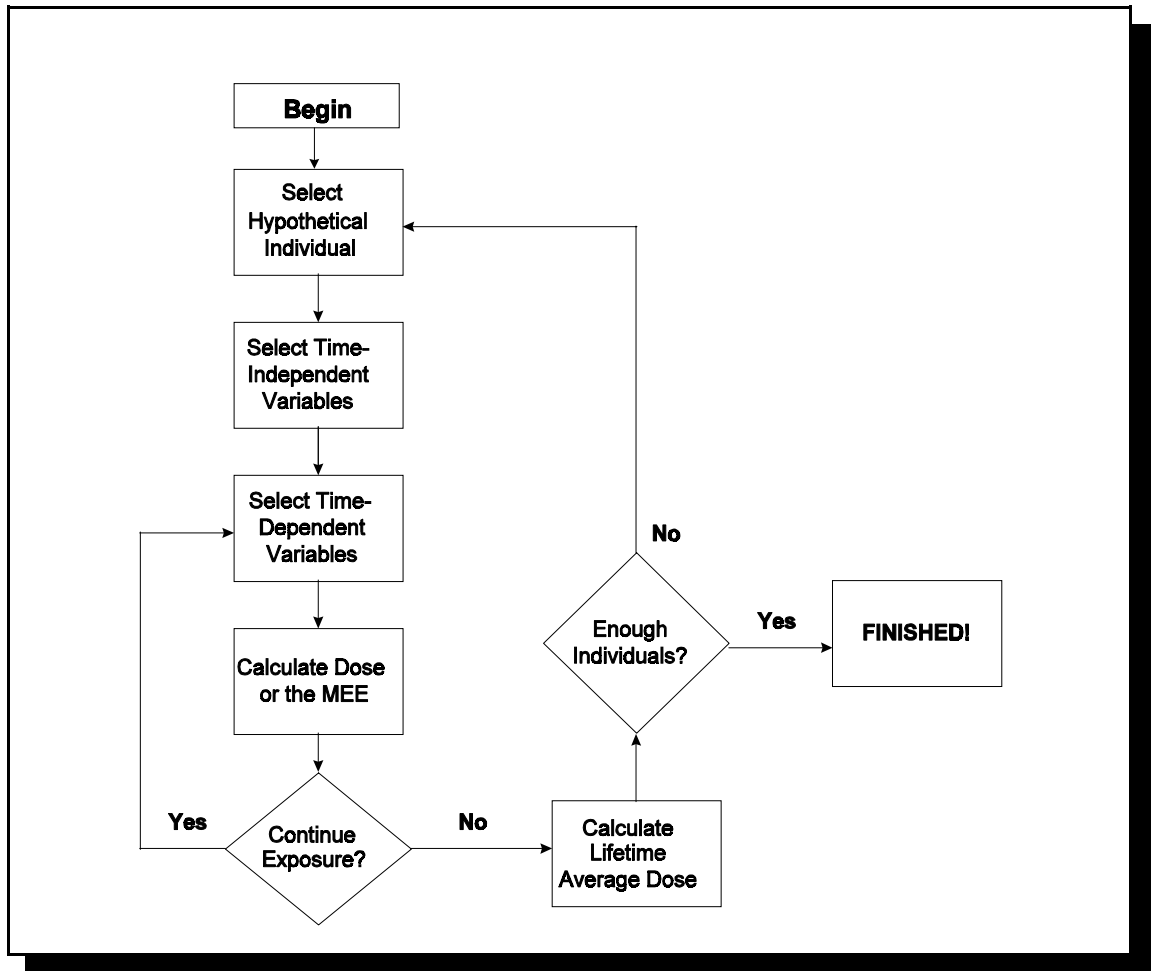


Figure D-5. Flowchart showing general approach for Microexposure Event (MEE) analysis.

Two important issues related to time step should be considered in implementing the MEE approach in PRA models. The first is the relationship between the length of the time step and the number of times random values are generated from a defined probability distribution. As the time step decreases, more time steps are needed to simulate exposures over a specified duration. For example, given a time step of one year and an exposure duration of 30 years, each random variable will be sampled 30 times (once per year); for a time step of one month and an exposure duration of 30 years, each random variable would be sampled 360 times (i.e., 12 months/year x 30 years). The Central Limit Theorem indicates that as n increases, the distribution of sample means is approximately normal, and the standard deviation of the sample distribution is inversely proportional to the square root of n . Thus a highly skewed input distribution (e.g., lognormal) may tend to become less skewed with increasing n (Figure D-6). A biased estimate of the RME risk in a PRA model may result if an inappropriately small or large time step is used in the model. This emphasizes the importance of having an empirical basis for selecting the time step and of exploring the time step as a variable in a sensitivity analysis of the model.

The second issue related to the time step concerns temporal correlations. Is it reasonable to assume that random values selected for consecutive time steps are completely independent? For example, consider body weight. The body weights of an individual measured at different times would be expected to show positive temporal autocorrelation; that is, body weight is likely to be similar (but not constant) from one time step to the next. For example, if an individual weighs 60 kg during one month, it is unlikely that they will weigh 80 kg the next month. If this scenario is accepted, then body weight should not be allowed to vary independently from one monthly time step to the next in the model. At shorter time steps, temporal correlation becomes more likely as a result of temporal autocorrelation. For example, one can expect a higher correlation between body weights on an individual measured on two successive days (one-day time step) than between weights measured at the midpoint of two successive years. Approaches to simulating temporal correlations in probabilistic models might include fixing an individual within a percentile range of a distribution (e.g., randomly assigned quartile) or using randomly assigned fluctuations (e.g., $BW_t = BW_{t-1} \pm x$).

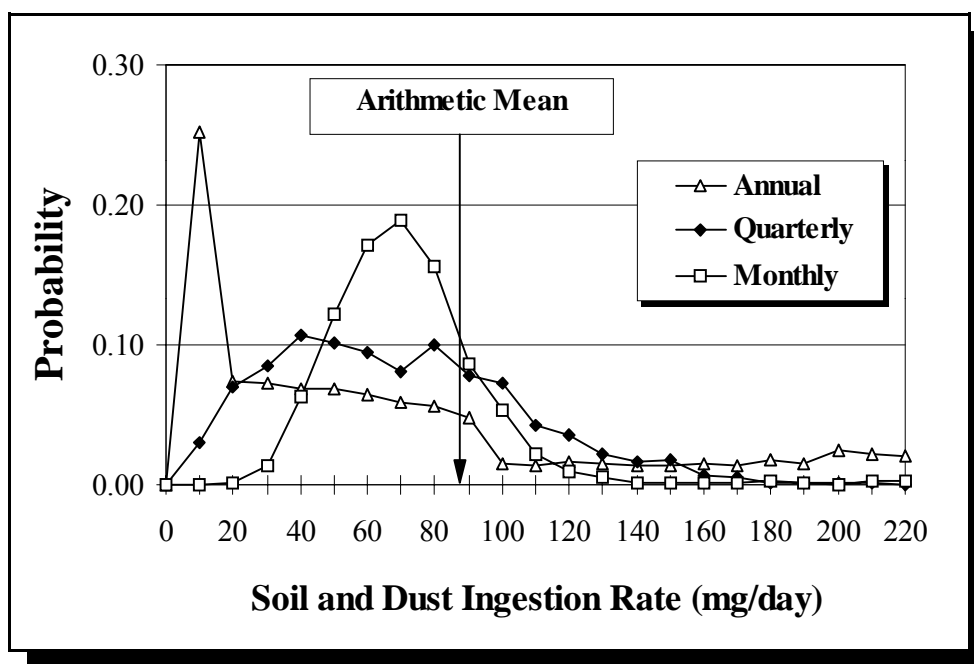


Figure D-6. Hypothetical example showing the effect of model time step on the probability distribution for soil and dust ingestion rate in children over a 1-year period. Number of samples (n) needed to simulate exposures: Annual (1), Quarterly (4), Monthly (12).

D.4.0 GEOSPATIAL STATISTICS

Spatial statistics is a specialized branch of statistics, falling under the heading of multivariate statistics, that explicitly takes into account the georeferenced or locational tagged context of data. Generally, environmental samples collected at Superfund sites have this geolocational information. By acknowledging the geography of site chemicals, information about the spatial distribution of contamination can be incorporated into an exposure assessment. In addition, knowledge about a receptors home range or patterns of movement may also be incorporated into the definition of the exposure unit (see Appendix C, Section C.2.0). Explicitly accounting for spatial relationships may lead to a more accurate estimate of the confidence limits for the arithmetic mean concentration. Geospatial statistics quantifies the spatial autocorrelation (Exhibit D-2) of sample measurements and allows for the exploration of the spatial distribution of exposure and risk using techniques of map generalization. By recording locational tags for each sample, information about spatial patterns within an exposure unit (EU) can be exploited to estimate both pre- and post-remediation exposure and risk.

In the past five years, with rapidly expanding software and hardware capabilities, some examples of the application of geostatistics can be found in exposure assessment and remedial design (e.g., Gomez-Hernandez, 1996; Goovaerts, 1996, 1997; Kriakidis, 1996; Ginevan and Splitstone, 1997; McKenna, 1998; Hope, 2000; 2001) as well as site assessment guidance (e.g., U.S. EPA, 2000).

Several important risk assessment issues are closely linked to geospatial statistics, as described in Exhibit D-3. Geospatial statistics comprises:

- *spatial autoregression*
- *geostatistics*
- *point pattern analysis*
- *image analysis*

The first three of these subjects can contribute to spatial statistical support of site risk assessments. The key concept linking all three is spatial autocorrelation, which refers to covariation among samples for a single chemical, or the tendency of data from locations that are relatively close together to be geographically correlated. By analogy, classical statistics treats soil samples as though they are balls, each having a battery of attributes, that can be placed into an

EXHIBIT D-2

POSITIVE SPATIAL AUTOCORRELATION

- Locations with a high value of Y tend to be surrounded by nearby high values of Y.
- Locations with a medium value of Y tend to be surrounded by nearby medium values of Y.
- Locations with a low value of Y tend to be surrounded by nearby low values of Y.

EXHIBIT D-3

EXAMPLES OF RISK ASSESSMENT ISSUES LINKED TO GEOSPATIAL STATISTICS

- Sampling tends to disproportionately represent “hot spots” (i.e., a relatively large portion of a data set with a small sample size (n) tends to be concentrated at “hot spots”).
- The upper confidence limit (UCL) for the arithmetic mean exposure concentration (e.g., chemical concentrations in soil) depends on the sample size.
- Additional sampling may be needed, especially to better define the spatial patterns or the extent of contamination.
- There is uncertainty about locations not sampled at a site, as well as uncertainty regarding the representativeness of neighboring samples in nearby EUs.

urn for statistical analysis; geospatial statistics treats soil samples as though they are clusters of grapes, with the branchy stems representing locational tags. Concentrations located on the same “branch” will be more strongly correlated than concentrations on different branches.

How is Geostatistics Different from Classical Statistics?

In general, geostatistics provides information beyond that provided by classical statistical techniques for at least two reasons. First, in classical statistics, observations are assumed to be independent. This assumption is often invalid at contaminated sites where the method by which a chemical is released into the environment (e.g., deposition from airborne emissions; migration of contaminant plume from a point source) often results in positive spatial autocorrelation (see Section D.4.1). In other words, observations located next to each other tend to contain similar levels of contamination (i.e., redundant information). For example, the higher the spatial autocorrelation, the less incremental information is provided by adding observations in close proximity to existing observations. This issue is compounded when the sample locations have been preferentially determined (e.g., “hot spot” sampling) rather than distributed at regular intervals or specified using random sampling methodology.

Second, geostatistics is able to use the geospatial information contained in the data to model uncertainty in contaminant concentrations for areas where data are scarce, a situation commonly encountered in site assessment work. Using geostatistics, information from samples collected from outside an EU can be used to model the uncertainty in the mean concentration within an EU. Approaches that do not consider the geospatial information present in the data are limited to the subset of samples within an EU.

D.4.1 CORRELATION AND SPATIAL AUTOCORRELATION

Several simple bivariate statistical approaches may be used to introduce the concept of spatial autocorrelation. Consider two variables, X and Y. For positive correlation there is a tendency for high values of X to be paired with the high values of Y, medium values of X to be with the medium values of Y, and low values of X with the low values of Y. The tendency is in the opposite direction for negative correlation; high values of X tend to be paired with low values of Y, and so on. Spatial autocorrelation, which virtually always is positive, directly parallels these definitions, but is written in terms of a single variable as shown in Exhibit D-2.

Just as the bivariate relationship between two variables, X and Y, can be portrayed by a scatter plot (Y versus X), the spatial autocorrelation relationship can be portrayed for a single variable, Y, (e.g., Y versus Y). A good example is the Moran scatterplot, which plots the sum or average of nearby values of Y versus Y. This plot is most effective when Y has been converted to z-scores. As shown in Figure D-7 and Section D.4.2, scatter plots can be used to illustrate some important issues related to sample size.

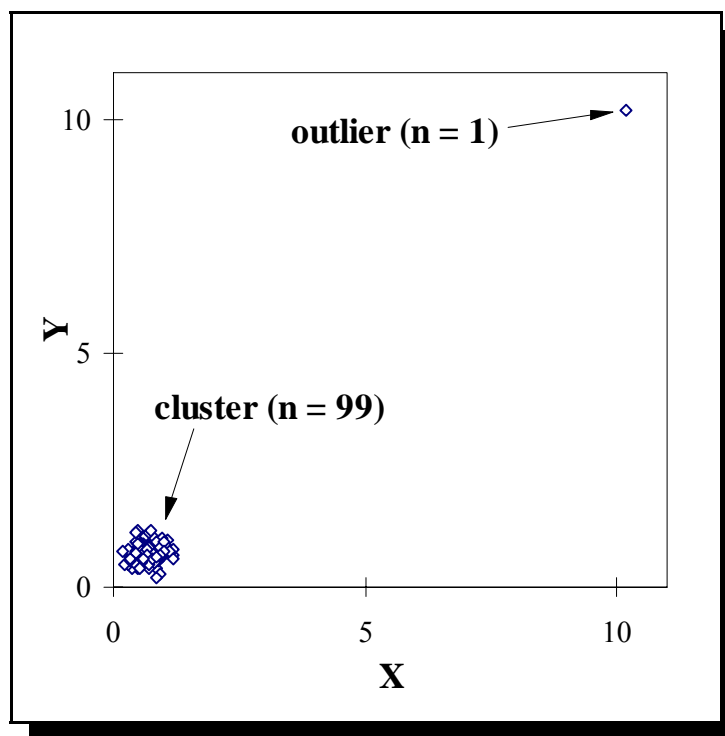


Figure D-7. Effect of an outlier on measured correlation: $r=0.956$ with outlier ($n=100$), whereas $r=0.086$ excluding outlier ($n=99$ clustered points).

If no soil samples were collected at a site ($n=0$), there is no information about the chemical concentrations in soil, and any guess may be considered an estimate. However, if the chemical concentration of a single sample ($n=1$) is measured, some information is obtained that partly restricts this estimate. As each additional independent sample is taken, more information is obtained, and the restriction on the estimate becomes more binding. If the same location is selected repeatedly for sampling, then the repeated measures, which may vary through time, will tend to be highly positively correlated; part of the information obtained from each sample is the same, and should not be counted more than once in estimating the site-wide soil concentration. Similarly, if immediately adjacent locations are sampled, the measures will often tend to be highly positively correlated (spatial autocorrelation). Once the first sample is taken, each additional sample provides only a fractional increment of new information about the site in its entirety.

D.4.2 EFFECTIVE SAMPLE SIZE (N^*) AND DEGREES OF FREEDOM

Repeated measures can result in data clustering, which can be illustrated in a scatter diagram. Because two points determine a straight line, if ($n-1$) points cluster together on a scatter diagram while a single additional point occurs far away from this cluster (i.e., an outlier), then the resulting bivariate correlation will be very high (see Figure D-7). This situation alludes to the notion of effective sample size (n^*): the n^* is no longer equal to the number of observations (n), but rather is dramatically reduced by the presence of inter-observational correlation. For the example shown in Figure D-7, n^* is slightly greater than 2 rather than 100 (i.e., n).

Spatial autocorrelation plays an analogous role in georeferenced data. If a sampling network is arranged as a 25-by-25 square grid (one sample point per grid cell), and superimposed over a large site so that a very large distance separates nearby sample locations, then essentially zero spatial autocorrelation should be present in the geographic distribution of the concentrations of any given chemical. Concentrations will appear to be haphazard across the site, rendering the effective sample size as $n^*=625$. If the distance between nearby locations on the sampling mesh is decreased so that the spatial correlation is only $r=0.050$, then the effective sample size decreases to $n^*=514$. The effect of reducing the inter-sample distance on spatial autocorrelation and n^* for a 25-by-25 grid is shown in Exhibit D-4. If r increases to 1, then n^* reduces to 1. Therefore, obtaining a measure of latent spatial autocorrelation is essential to estimating n^* ; this in turn is critical to determining confidence limits

for estimates of mean concentrations, which are sensitive to sample size. The UCL for the mean will be biased *only* when very high levels of spatial autocorrelation are present; this is because the Student-t statistic used to estimate the UCL (assuming a normal distribution) changes very little as the degrees of freedom (related to sample size) increases above 10; part of the difference between n and n^* is offset by an inflation of the variance.

EXHIBIT D-4	
EFFECT OF SPATIAL AUTOCORRELATION (r) ON EFFECTIVE SAMPLE SIZE (n^*)	
r	n^*
0.000	625
0.050	514
0.539	64
0.957	3
1.000	1

The concept of effective degrees of freedom is important in exposure assessment because high positive spatial autocorrelation can bias the estimate of the UCL concentration if geospatial statistics are not considered. This should be of particular concern when specific locations at a site are intensively sampled (e.g., suspected “hot spots”), and other locations are relatively undersampled. Accordingly, the design of the sampling network itself can be evaluated from the perspective of geospatial statistics in order to ascertain the quality of sample information. The ideal sampling network should provide geographic representativeness, should be roughly uniformly distributed over a site, and is best implemented as a stratified random sampling design; that is, the site is partitioned into geographic stratum (e.g., EUs), and then a random sampling of points is selected within each strata. In practice, sample designs may need to focus on objectives that are in conflict with the above ideals. For example, intense sampling of suspected “hotspots” may be necessary at some sites, at the expense of a more representative spatial coverage of the site. In such cases, several statistical techniques are available for assessing the statistical benefit (in terms of reducing uncertainty) of additional sampling at undersampled locations.

D.4.3 ASSESSMENT OF ADDITIONAL SITE SAMPLING

Thiessen Polygons. In addition to calculating nearest neighbor statistics, the adequacy of a sampling network can be assessed by Voronoi (i.e., Thiessen polygon) surface partitioning, a popular approach used in mapping intra-site geographic distributions. This procedure divides a site into a mutually exclusive set of polygons, each polygon containing a single measured concentration. Each polygon has the unique property that any location within the polygon is closer to the polygon’s sample location than to any other sample point (Clifford et al., 1995). The concentration measured at the sample

point in the polygon is assigned to the entire area of the polygon. The intensity of sample points on a surface can be measured by Equation D-3 mean inverse polygon areas:

$$SI = \frac{1}{m} \sum_{i=1}^m A_i^{-1} \quad \text{Equation D-3}$$

where SI is a measure of the sampling intensity, A_i is the area of the i^{th} polygon, and m is the number of interior polygons (those not along the edge of the site); $m < n$. The variance of the sampling intensity can be expressed by Equation D-4:

$$SI_{\text{Variance}} = \frac{1}{m-1} \left[\sum_{i=1}^m A_i^{-2} - \frac{1}{m} \left(\sum_{i=1}^m A_i^{-1} \right)^2 \right] \quad \text{Equation D-4}$$

If the sampling network is uniform (i.e., polygon areas are equal), the variance will be essentially zero. The variance will increase as the network deviates from uniform. This measure can be used to assess whether or not additional samples will improve the spatial coverage.

☞ Sampling locations that would yield a dramatic reduction in the variance should be given priority for future sampling efforts.

Thiessen polygons can be used to develop area-weighted estimates of the arithmetic mean concentration ($C_{\text{soil,w}}$) according to the following general equation:

$$C_{\text{soil,w}} = \sum_{i=1}^n C_i \frac{A_i}{A_T} \quad \text{Equation D-5}$$

where C_i is the concentration in the i^{th} polygon, A_i is the area of the i^{th} polygon in the EU, and A_T is the total area of the EU. The weight for each measurement is essentially the ratio of the area of each polygon to the total area of the site. Clifford et al. (1995) applied this approach to an ecological risk assessment of the burrowing owl with the following simplifying assumptions: habitat range is circular, size of EU is constant (75 ha) although location may vary, and organisms spend equal time in all portions of their habitat. Given these assumptions, a nonparametric bootstrap method can be used to determine the approximate 95% UCL for the mean concentration (see Appendix C). Using Monte Carlo analysis, $C_{\text{soil,w}}$ can be estimated for different locations of the EU according to Equation D-5, and confidence limits can be generated from the multiple bootstrap estimates. Burmaster and Thompson (1997) demonstrate a similar approach in which the EU (with constant area but random rectangular dimensions) is overlaid on the Thiessen polygon surface and 95% UCL for the mean is calculated from the bootstrap sample.

Linear Regression. Another diagnostic is found in the linear regression literature. The locational tag coordinates (e.g., longitude, latitude) can be converted to z-scores (say z_u and z_v) for the following calculation:

$$Y = \frac{1}{n} + \frac{z_u^2 + z_v^2 - 2r_{uv}z_u z_v}{(n-1)(1-r_{uv}^2)} \quad \text{Equation D-6}$$

where Y is a measure of the sampling network, r_{uv} is the correlation between the coordinate axes, and n is the number of samples. Any sampling location (z_u, z_v) in which $Y > 9/n$ may be considered too isolated in the sampling network. Additional sampling locations would be positioned closer to it to improve the overall coverage of the sampling network.


D.4.4 MAP GENERALIZATION

Another important application of geospatial statistics to risk assessment is that of map generalization, which draws on the subjects of geostatistics and spatial autoregression. Techniques developed for both topics exploit spatial autocorrelation in order to produce a map.

Kriging and Semivariograms. Geostatistics may employ kriging, which yields statistical guesses at values of a chemical at unsampled locations based on information obtained from sampled locations. Kriging assumes that the underlying geographic distribution is continuous, evaluates spatial autocorrelation in terms of distance separating sample points, and employs a scatter diagram similar to the Moran scatter plot to portray this relationship (i.e., the semivariogram plot: half the squared difference between measured concentrations for two sampled locations versus distance separating these two locations). The best-fit line to this scatter of points is described by one of about a dozen equations (semivariogram models).

Many different kriging approaches can be applied to quantify the spatial relationships among geographic attributes within an exposure unit. For example, site-specific chemical concentrations may be correlated with geologic information, such as glacial deposits, soil characteristics of core samples, and attributes that represent favorable habitats for ecological receptors. This information can be used to expand the available data and improve estimates of chemical concentrations at unsampled locations by employing a technique called co-kriging.

Thiessen Polygons and Spatial Autoregression. Spatial autoregression assumes a discretized surface, uses the Thiessen polygon surface partitioning to construct a Moran scatter plot, and can be used to estimate values at selected points with a regression-type equation. Theoretically, the exponential semivariogram model relates to the conditional autoregressive model, and the Bessel function semivariogram model relates to the simultaneous autoregressive model; in practice, though, the spherical semivariogram model often provides the best description of a semivariogram plot. Regardless of which approach is taken to map generalization, one relevant contribution of these two subjects is the following observation:

 *Including positive spatial autocorrelation results in more accurate variance estimates; this in turn yields more accurate estimates of the 95% UCL for the mean concentration.*

D.4.5 IMPLEMENTATION ISSUES RELATED TO GEOREFERENCED DATA

Estimation of parameters, for either geostatistical or spatial autoregressive models, cannot be achieved with ordinary least squares (OLS) techniques; nonlinear least squares must be used. While OLS provides unbiased regression coefficients, these estimates are not necessarily sufficient (i.e., they do not summarize all of the information in a sample pertaining to the population), efficient (i.e., the standard errors often are incorrect), and consistent (i.e., the asymptotic sampling distribution concentration will not be at the parameter value). In other words, OLS essentially uses the wrong degrees of freedom in its calculations, as described in Section D.4.2. Two additional complications of georeferenced data that do not appear in other types of data are (1) spatial autocorrelation might be directional (i.e., directional dependency); and (2) variance might be nonconstant over space as well as over the magnitude of the dependent variable, Y (e.g., chemical concentration). Several statistical approaches, which are beyond the scope of this guidance, are available for analyzing these potential sources of bias in the exposure concentration estimates (Isaaks and Srivastava, 1989; Cressie, 1991; Griffith, 1993; Ginevan and Splitstone, 1997).

D.5.0 EXPERT JUDGMENT AND BAYESIAN ANALYSIS

Up to this point in RAGS Volume 3: Part A, risk has been characterized as having a population probability distribution with parameters (e.g., mean, standard deviation) that can, theoretically, be estimated from observation. In theory, risk estimates could be derived by repeatedly measuring risk in subsets of the population of interest (e.g., repeated measurements of site-related cancer risk). The unstated expectation, or goal, is that the PRA model will accurately simulate this *real* risk distribution. This approach derives from a *classical* view of probability. The *classical* or *frequentist* view defines the probability of an event as the frequency with which it occurs in a long sequence of similar trials. From the *frequentist* perspective, the probability of having a flipped coin land *heads-up* is given by the frequency distribution of heads-up results derived from repeated similar trials of coin flips. For real-world decisions such as those informed by Superfund risk assessments, there is uncertainty that the sample data are representative of the population (see Chapter 1, Section 1.2.4).

Bayesian View of Probability. A Bayesian perspective on probability allows distributions to be constructed based on the judgment of an expert in the field. The subjectivist or Bayesian view is that the probability of an event occurring is the degree of belief a person has in the occurrence. Probabilities can be assessed by experts using scientific knowledge, judgment, data, past experience, and intuition. Different people may assign different probabilities to an event, and a single individual may assign different probabilities to the same event when considered at different times. The consequence is that probabilities become conditional and the conditions must be explicitly stated (Howson and Urbach, 1989; Morgan and Henrion, 1990; Ott, 1995; Sivia, 1996). These conditional probabilities can, of course, be updated with new information.

Using the coin flip analogy above, a Bayesian perspective might be that, based on experience with coins, assuming that most coins are *fair*, and that a fair coin would be expected to land heads-up half the time, the expected probability of the tossed coin landing heads-up is 0.5. If the outcome of repeated trials was different from the expected, the Bayesian approach would be to update the probability based on the new data. In the coin flip example, both the Bayesian and frequentist approaches will arrive at the same conclusions, because the outcome is amenable to rigorous experimentation. Where the two approaches can be expected to differ is in the assignment of probabilities to events that cannot be rigorously measured; for example, the probability of a site-related cancer risk, or the probability of a child ingesting a specific amount of soil.

The subjective judgment of experts is, therefore, an important tool in the Bayesian approach to risk assessment. For example, the input distributions for a PRA may be based upon the judgment of one or more experts who rely upon estimates from the literature, data from experimental studies, and any other information they consider relevant. Even when formal elicitations of expert opinion are not done, the final selection of the form and parameters of the input distributions usually involves some subjective judgment by the analyst. One of the challenges of incorporating judgments from experts or lay people is that there can be overconfidence bias (i.e., people tend to underestimate their uncertainty). There is a rich literature about the protocol for conducting expert elicitations and using the results to support decisions (Lichtenstein and Fischhoff, 1977; Morgan and Henrion, 1990; Shlyakhter and Kammen, 1992). Elicitation of expert judgment has been used to obtain distributions for use in risk assessments (Morgan and Henrion, 1990; Hora, 1992; U.S. EPA, 1997;) and in developing air quality standards (U.S. EPA, 1982).

In addition to providing input distributions for PRAs, Bayesian analysis allows the current state of knowledge, expressed as a probability distribution, to be formally combined with new data to reach an updated information state. The distribution expressing the current knowledge is the *prior distribution* and may be the output of a PRA (Figure D-8). An appropriate *likelihood function* for the data must also be formulated. The likelihood function is based upon an understanding of the data gathering process and is used to determine the probability of observing a new set of data given that a particular risk estimate is true.

EXHIBIT D-5

COMPONENTS OF BAYES THEOREM IN PRA

- Input probability distributions for exposure (or toxicity) based on available data or expert judgment
- Prior probability distribution for risk based on input probability distributions (output from PRA)
- New data
- Likelihood function, expressing the probability of observing the new data conditional on prior risk estimates
- Posterior (updated) probability distribution for risk

Once the prior distribution is determined, the new data values are collected, and the likelihood function is assumed, Bayes theorem (Exhibit D-5) provides a systematic procedure for updating the probabilistic assessment of risk. The updated information state is called the *posterior distribution* and reflects the reduction in uncertainty arising from the new information.

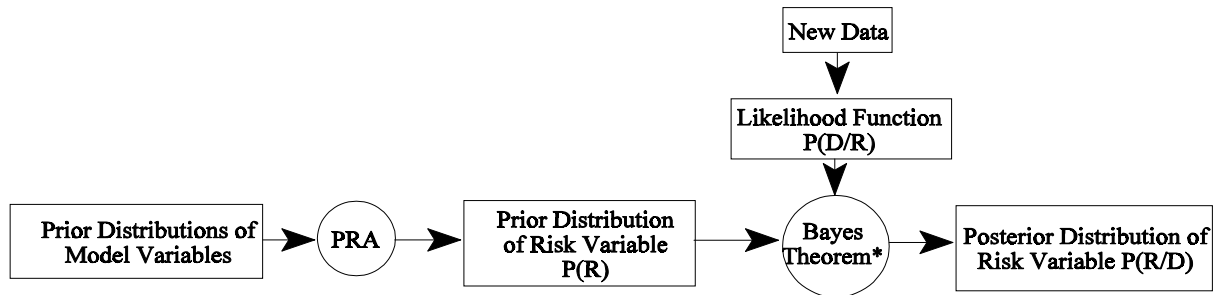


Figure D-8. Conceptual model of Bayesian Monte Carlo analysis. A PRA simulation yields a prior distribution of risk based on probability distributions for input variables. Given new data for an input variable, and a likelihood function for risk, Bayes Theorem (Eq. D-7) can be used to generate a posterior distribution of risk. The expression $P(D/R)$ refers to a conditional probability, “the probability of D , given R ”. Conditional probabilities can be thought of as relative frequencies, where R is the information given, and D is the event being computed when a particular value of R occurs.

$$\text{Bayes Theorem}^*: \quad P(R_i/D) = \frac{P(D/R_i) P(R_i)}{\sum_{j=1}^N P(D/R_j) P(R_j)} \quad \text{Equation D-7}$$


- D = new data
- R_i = i^{th} risk prediction associated with new data
- R_j = j^{th} risk estimate simulated from PRA model
- N = number of risk estimates from the PRA model

For example, suppose a model is available to relate soil tetrachlorodibenzodioxin (TCDD) concentrations at a site with serum concentrations of TCDD. A probability distribution of soil concentrations is created based upon expert judgment and a limited amount of site specific data. Using the model, the soil concentrations can be associated with a distribution of serum TCDD concentrations (P^R), the prior distribution). New site-specific data (D) are subsequently collected on serum TCDD concentrations in order to reduce uncertainty in the risk estimate. Assume that it is known that serum TCDD concentrations generally follow a lognormal distribution and that the best estimate of the parameters of this distribution come from the prior distribution on serum TCDD. This creates the likelihood function ($P(D|R)$). Using Bayes Theorem, the new data are used to form a revised distribution of serum TCDD. This is the posterior distribution ($P(R|D)$).

Bayesian Monte Carlo analysis. In the past, the use of Bayesian analysis was limited by the degree of mathematical complexity involved. Using Monte Carlo analysis to carry out the PRA, rather than mathematical equations to describe the distributions, allows the calculations to be done much more easily. This variation on traditional Bayesian methods is called Bayesian Monte Carlo analysis (Patwardan and Small, 1992; Dakins et al., 1996). In the TCDD example discussed above and illustrated in Figure D-7, the required calculations are carried out for each of the N iterations of the Monte Carlo analysis (I and j go from 1 to N).

Bayesian Monte Carlo analysis is appropriate in several situations. If a model has been created and a distribution developed using PRA, new information may be incorporated without the need to repeat the entire analysis. This information could be on one of the uncertain parameters of the model or on the model output variable. Similarly, a generalized risk model with generic parameter distributions may be used for a Superfund risk assessment with the model predictions fine-tuned using data from a particular site of interest. Finally, after a distribution is developed, the amount of uncertainty that exists may be too large for the risk manager to make a decision. In this case, the risk manager might seek out new information that would refine the analysis and decrease the uncertainty.

Bayesian Monte Carlo analysis can also be combined with techniques from decision analysis to help determine the type and quantity of data that should be collected to reduce uncertainty. Decision analysis is a technique used to help organize and structure the decision maker's thought process and identify a best strategy for action. To determine the appropriate action, one defines the range of possible decisions, evaluates the expected value of the utility or loss function associated with each decision, and selects the decision that maximizes the expected utility or minimizes the expected loss.

 *Decision analysis provides a quantitative approach for evaluating the benefits of including an expanded assessment of uncertainty and the subsequent benefits of reducing this uncertainty.*

Value of Information. Value of information (VOI) analysis involves estimating the value that new information can have to a risk manager before that information is actually obtained (Clemen, 1996). It's a measure of the importance of uncertainty in terms of the expected improvement in a risk management decision that might come from better information. Examples of VOI quantities are the expected value of including uncertainty (EVIU), the expected value of sample information (EVSI), the expected value of perfect information (EVPI). Calculation of these quantities can be done using mathematical methods, numerical integration (Finkel and Evans, 1987), or Monte Carlo techniques (Dakins, 1999)

Value of information calculations require the specification of either a utility or a loss function. A loss function states the losses associated with making different types of decision errors including both direct monetary costs and losses associated with other consequences. Loss functions take various forms depending on the risk management situation (Morgan and Henrion, 1990).

Expected Value of Including Uncertainty. The expected value of including uncertainty, EVIU, is a measure of the value of carrying out a PRA. It's the difference between the expected loss of a decision based on a point estimate risk assessment and the expected loss of the decision that considers uncertainty (Figure D-9). If uncertainty in a risk assessment has been estimated using Monte Carlo techniques and a loss function has been specified, the EVIU can be easily calculated. First, the management decision from the point estimate assessment is determined. The loss from making this decision is calculated for each iteration of the Monte Carlo, each time assuming that the risk estimate from that iteration is true. The expected loss is the average of these individual losses. The expected loss for the PRA is determined by calculating the expected loss for a full range of management decisions and selecting the decision with the lowest expected loss. The EVIU is calculated by subtracting the loss associated with the PRA from that associated with the point estimate risk assessment.

Expected Value of Sample Information. The expected value of sample information is the difference between the expected loss of the decision based on the PRA and the expected loss of the decision from an improved information state. As such, the EVSI is a measure of the value that may result from the collection and use of new information (Figure D-9). Calculation of the EVSI involves a technique called preposterior analysis and is somewhat more complicated.

This type of analysis is termed "preposterior" because it involves the possible posterior distributions resulting from potential samples that have not yet been taken. For each replication from the Monte Carlo simulation, the predicted value from the model is used to randomly generate a set of K data points. Each set of data points is then used to calculate the posterior probabilities for the N Monte Carlo simulated values. These posterior probabilities are then used to obtain the optimal answer to the management question at this new level of uncertainty by selecting the decision that minimizes the expected loss over all possible management decisions.

This procedure is repeated for each of the N replications of the Monte Carlo analysis resulting in N posterior distributions, N management decisions, and N associated expected losses. Because each of these outcomes is equally weighted, the expected loss associated with the state of uncertainty expected to exist after the data collection program is carried out is simply the average of the N expected losses. The EVSI is the difference between the expected loss based on the results of the PRA and the expected loss from the updated information state.

Expected Value of Perfect Information. The EVPI is the difference between the expected loss of the decision based on the results of the PRA and the expected loss of the optimal management decision if all uncertainty were eliminated. In actual application, no research plan or data collection program can completely eliminate uncertainty, only reduce it. The EVPI is an upper bound for the expected value of efforts to reduce uncertainty and so provides the ultimate bound on what should be spent on research and data collection efforts.

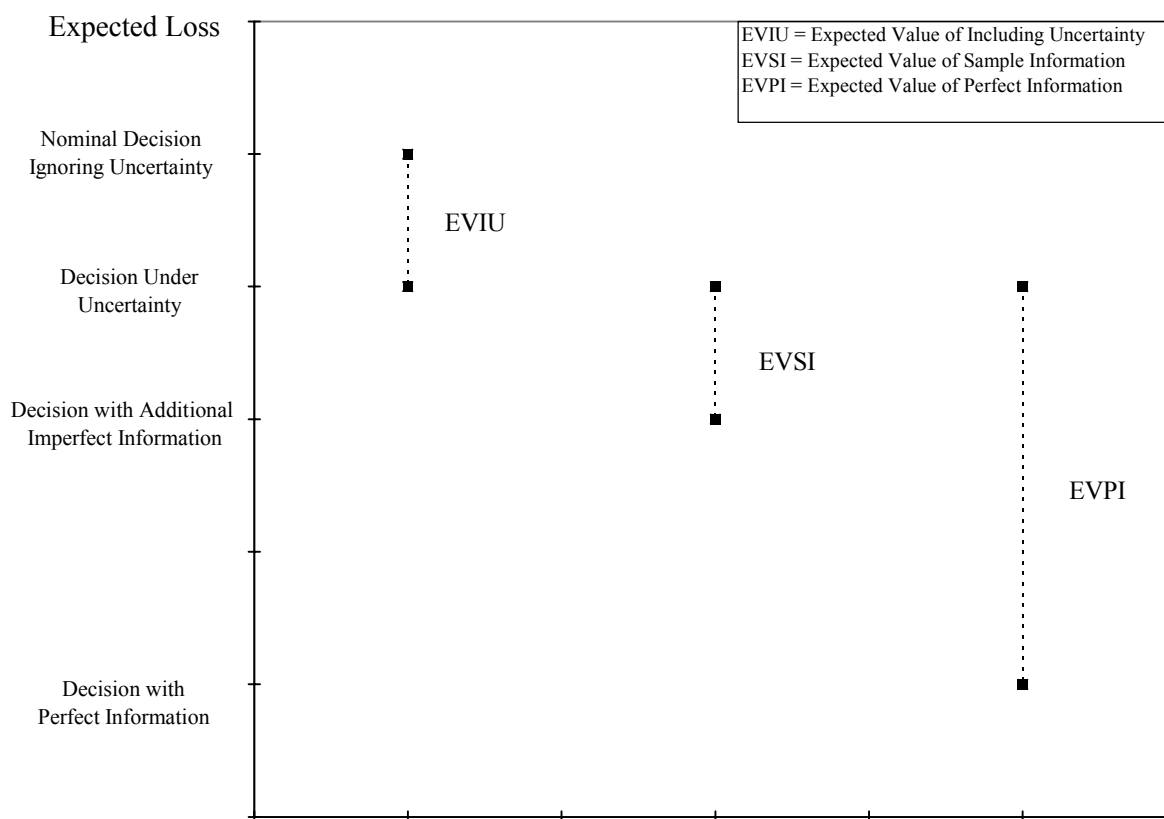


Figure D-9. Expected Loss associated with various types of information incorporated into a generic uncertainty analysis. The x-axis reflects different categories of value of information (VOI) quantities. The y-axis reflects the increasing Expected Loss with increasing uncertainty.

When a PRA has been carried out using Monte Carlo techniques, the expected loss associated with perfect information is calculated by determining the expected loss for each iteration of the Monte Carlo, assuming that the correct management decision, if that iteration were true, is made. As always, the expected loss is the average of these losses, and the EVPI is calculated by subtraction.

Uses of Value of Information in Risk Assessment. VOI analysis has many benefits for risk managers. First, VOI analysis makes the losses associated with decision errors explicit, balances competing probabilities and costs, and helps identify the decision alternative that minimizes the expected loss. VOI analysis can help a decision maker overcome a fear of uncertainty by developing a method to handle it. If the losses associated with making a poor decision are unclear, small uncertainties can take on major importance. Conversely, if the losses associated with different risk management decisions are similar, little additional effort need be expended to continue to consider the alternatives.

In addition, VOI analysis helps prioritize spending on research. It provides insights into how resources could be spent to achieve the most cost-effective reduction in uncertainty by identifying which sources of uncertainty should be reduced, what type of data should be obtained, and how much data is

needed. Finally, VOI analysis may help decision makers explain the rationale for their decisions to the public and help the public understand the multiple objectives considered in managing risks.

Expected Loss is usually greatest when uncertainty in risk estimates is ignored. For example, by quantifying uncertainty in risk (e.g., 2-D MCA, Bayesian Monte Carlo analysis) a risk manager may determine that the cleanup level associated with the 90th percentile of the risk distribution (rather than the 95th percentile) is adequately protective. Quantifying uncertainty may also result in lower expected loss when more soil remediation is required due to the losses associated with possible under-remediation, e.g., cost of additional sampling or lost revenue due to failure to meet land use requirements. The expected loss may be further reduced by collecting additional soil samples, which would presumably reduce uncertainty in estimates of mean exposure point concentrations. The expected loss may be minimized by obtaining "perfect" information (i.e., no uncertainty); however, as shown in Figure D-9, EVPI spans a wide range of expected loss because the value associated with reducing uncertainty may be tempered by costs associated with additional sampling and analysis. In practice, risk assessors consider this issue when deciding to obtain additional samples for site characterization.

The decision to obtain additional information in order to reduce uncertainty should be made on a site-specific basis, taking into account the potential impact that reducing uncertainty may have on the overall remedial decision. Important questions to consider include: (1) Are the risk estimates sufficiently sensitive to an exposure variable that collecting further data will reduce uncertainty? and (2) Are the confidence limits on the 95th percentile risk estimate sufficiently wide that reducing uncertainty may alter the cleanup goal? An example of decision framework applicable to PRA is presented in Figure D-10. The framework has three tiers. Tier 1 includes the point estimate approach and an assessment of the need for PRA. In Tier 2, the EVIU is calculated and, if warranted, a PRA is conducted. In Tier 3, the value of additional information is assessed and Bayes Theorem would be used to incorporate the new information and update probability distributions.

Limitations of These Techniques. Figure D-10 illustrates situations where Bayesian analysis and value of information quantities may not be helpful. For example, if point estimate risk assessment is selected as the appropriate method, these techniques do not apply. In addition, as site-specific data become available that are increasingly comprehensive and representative of the population of interest, Bayesian Monte Carlo analysis and the Monte Carlo analysis using the classical (frequentist) methods will approach the same result. This is because the site-specific data are incorporated into both approaches. To be representative and comprehensive, the data set must be sufficiently large, randomly selected, and represent the full range of variability that exists in the population (e.g., temporal, spatial, inter-individual). However, data sets are rarely perfect, often too small, suffer from relatively high sampling and/or measurement errors, or don't represent the entire population variability over time, space, age, gender, or other important variables. If the data cannot be assumed to describe the population distribution sufficiently well, then PRA will help to more fully develop the entire range of the population distribution and the Bayesian Monte Carlo analysis will act to refine the model estimates.

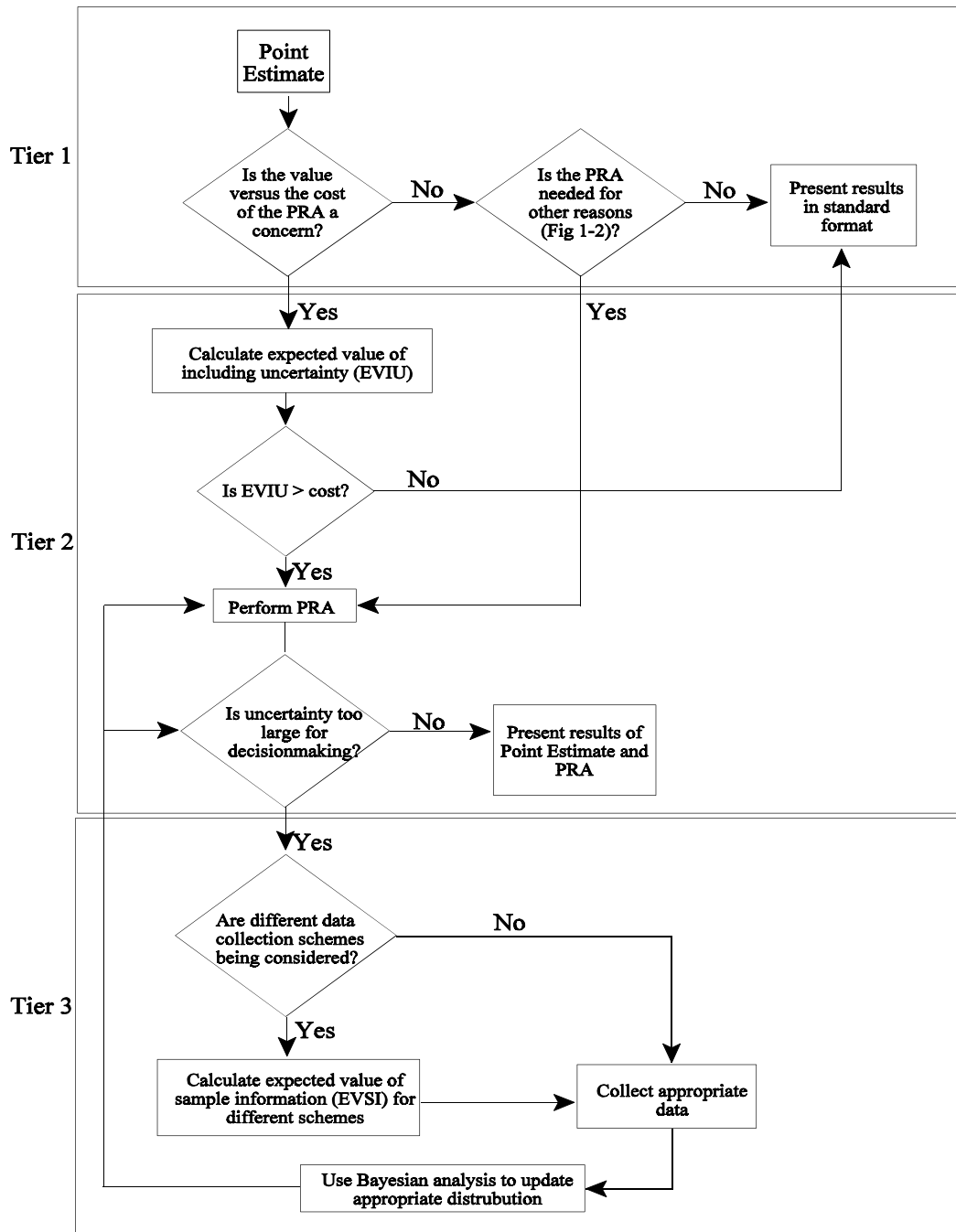


Figure D-10. Conceptual model for evaluating the expected value of including uncertainty in a Bayesian Monte Carlo analysis.

In order to carry out VOI calculations, a loss function must be assumed. Definition of the loss function may be complex due to multiple decision goals and/or multiple decision makers and may be difficult to capture in an equation. Finally, for Bayesian analysis and the calculation of the EVSI to be helpful, one or more sources of new data must exist. In addition, some information must be available about these data since a likelihood function describing its probability distribution must be assumed.

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